=> d his

(FILE 'HOME' ENTERED AT 13:49:37 ON 16 NOV 2006)

FILE 'REGISTRY' ENTERED AT 13:49:58 ON 16 NOV 2006

L1 STRUCTURE UPLOADED

L2 2 S L1

L3 8 S L1 FULL

FILE 'HCAPLUS, CHEMCATS' ENTERED AT 13:50:50 ON 16 NOV 2006

L4 2 S L3

FILE 'HCAPLUS, HCAOLD, USPATFULL, EPFULL, BIOSIS, MEDLINE' ENTERED AT 13:51:47 ON 16 NOV 2006

L5 188036 S BENZOIC ACID? OR BENZOIC ACID DERIVATIVE?

L6 103714 S L5 AND ?AMINO?

L7 680313 S DIABETES OR INSULIN RESISTANCE OR PEROXISOME PROLIFERATOR-ACT

L8 10162 S L6 AND L7

L9 4662 S L8 AND LIPID?

L10 4647 S L9 AND (PHARMACEUTICAL OR TREAT? OR COMPOSITION)

L11 4406 S L10 AND (SALT OR PRODRUG)

L12 3284 S L11 AND (OXY OR SULFUR OR SULFONYL)

L13 901 S L12 AND ORTHO

L14 508 S L13 AND (PHENOXY OR OXOETHYL OR OXOPROPYL)

L15 487 S L14 AND BENZYL

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 ST

G1 X, Cb, Cy, Hy, Ak

Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 15:23:43 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 138 TO ITERATE

100.0% PROCESSED 138 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 2056 TO 3464

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 15:23:46 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 3141 TO ITERATE

·100.0% PROCESSED 3141 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

L3 0 SEA SSS FUL L1

=>

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1

STR

G1 0,S

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 13:50:17 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 8 TO ITERATE

100.0% PROCESSED

8 ITERATIONS

2 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:

ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

8 TO 329

PROJECTED ANSWERS:

2 TO 124

L2

2 SEA SSS SAM L1

=> d scan

L2 2 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Benzoic acid, 2-[[[4-[2-[ethyl[[4-(trifluoromethyl)phenyl]methyl]amino]-2oxoethyl]phenyl]thio]methyl]- (9CI)

MF C26 H24 F3 N O3 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 2 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Benzoic acid, 2-[[4-[2-[hexyl(phenylmethyl)amino]-2-oxoethyl]-2-

10/518,007

methoxyphenoxy] methyl] - (9CI) MF C30 H35 N O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> s l1 full FULL SEARCH INITIATED 13:50:33 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED -74 TO ITERATE

74 ITERATIONS 100.0% PROCESSED

8 ANSWERS

SEARCH TIME: 00.00.01

L3 8 SEA SSS FUL L1

=> d scan

8 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN L3

Benzoic acid, 2-[[4-[2-[ethyl[(2-fluorophenyl)methyl]amino]-2-IN oxoethyl]phenoxy]methyl]- (9CI)

C25 H24 F N O4 MF

$$CO_2H$$
 CH_2-O
 CH_2
 CH_2
 CH_2
 CH_2
 CH_2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):7

REGISTRY COPYRIGHT 2006 ACS on STN 8 ANSWERS

Benzoic acid, 2-[[4-[2-[hexyl(phenylmethyl)amino]-2-oxoethyl]-2-IN methoxyphenoxy]methyl] - (9CI)

C30 H35 N O5 MF

10/518,007

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 8 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

Benzoic acid, 2-[[4-[2-[[(2,4-difluorophenyl)methyl]heptylamino]-2-oxoethyl]phenoxy]methyl]- (9CI)

MF C30 H33 F2 N O4

$$CH_2-O$$
 CH_2-C-N
 CH_2
 C

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 8 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Benzoic acid, 2-[[[4-[2-[[(4-chlorophenyl)methyl]ethylamino]-2oxoethyl]phenyl]thio]methyl]- (9CI)

MF C25 H24 C1 N O3 S

$$CO_2H$$
 CH_2-S
 $CH_2-C-N-CH_2$
 CH_2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 8 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Benzoic acid, 2-[[[4-[2-[[(2,4-difluorophenyl)methyl]heptylamino]-2oxoethyl]phenyl]thio]methyl]- (9CI)

MF C30 H33 F2 N O3 S

$$CH_2-S$$
 CH_2-C-N
 CH_2
 C

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 8 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Benzoic acid, 2-[[[4-[2-[ethyl[[4-(trifluoromethyl)phenyl]methyl]amino]-2oxoethyl]phenyl]thio]methyl]- (9CI)

MF C26 H24 F3 N O3 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 8 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

MF . C29 H32 F N O4

Me- (CH₂)₅-N-C-CH₂

Ph-CH₂

$$O$$

HO₂C

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 8 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

Benzoic acid, 2-[[4-[2-[hexyl(phenylmethyl)amino]-2-oxoethyl]phenoxy]methyl]- (9CI)

MF C29 H33 N O4

IN

$$CO_2H$$
 CH_2-O
 CH_2-Ph
 $CH_2-C-N-(CH_2)_5-Me$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> file hcaplus chemcat
COST IN U.S. DOLLARS

COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
166.94
167.15

FILE 'HCAPLUS' ENTERED AT 13:50:50 ON 16 NOV 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'CHEMCATS' ENTERED AT 13:50:50 ON 16 NOV 2006
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COPYRIGHT (C) 2006 American Chemical Society (ACS)

=> s 13 L4 2 L3

=> d 1-2 ibib abs hitstr

L4 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:2838 HCAPLUS

DOCUMENT NUMBER: 140:41910

TITLE: Preparation of ortho-substituted benzoic acid

derivatives for the treatment of insulin resistance

INVENTOR(S): Li, Lanna

PATENT ASSIGNEE(S): Astrazeneca Ab, Swed. SOURCE: PCT Int. Appl., 60 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.				KINI	DATE AP			APPL	PPLICATION NO.				DATE			
WO 2004000790			A1		20031231		WO 2003-GB2584					20030617				
W:	ΑE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,
	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	ΚP,	KR,	KZ,	LC,	LK,	LR,
	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NI,	NO,	NZ,	OM,
	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	TJ,	TM,	TN,	TR,
	TT,	TZ,	UA,	ŪĠ,	US,	UZ,	VC,	VN,	ΥU,	ZA,	ZM,	ZW				
RW:	GH,	GM,	ΚE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	ŪĠ,	ZM,	ZW,	AM,	ΑZ,	BY,
	KG,	ΚZ,	MD,	RU,	ΤJ,	TM,	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,
	FI,	FR,	GB,	GR,	HU,	ΙE,	IT,	LU,	MC,	NL,	PT,	RO,	SE,	SI,	SK,	TR,
,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG

_	2489834		AA	20031231	CA 2003-2489834		20030617		
CA	2489834		С	20061003					
ΑŪ	200324009	9	A1	20040106	AU 2003-240099		20030617		
BR	200301193	2	Α	20050322	BR 2003-11932		20030617		
EP	. 1517883		A1	20050330	EP 2003-732713		20030617		
	R: AT,	BE, CH,	DE,	DK, ES, FR,	GB, GR, IT, LI, LU,	NL, S	SE, MC, PT,		
	IE,	SI, LT,	LV,	FI, RO, MK,	CY, AL, TR, BG, CZ,	EE, H	HU, SK		
CN	1675171		Α	20050928	CN 2003-819474		20030617		
JP	200552997	0	T2	20051006	JP 2004-515007		20030617		
JP	3782818		B2	20060607					
МО	200400535	3	A	20050120	NO 2004-5353		20041207		
US	200525619	8	A1	20051117	US 2004-518007		20041214		
ZA	200401016	1	A	20051020	ZA 2004-10161		20041215		
JP	200618278	2	A2	20060713	JP 2006-19068		20060127		
PRIORITY	APPLN. I	NFO.:			SE 2002-1935	Α	20020620		
					SE 2002-3826	Α	20021220		
					JP 2004-515007	A3	3 20030617		
					WO 2003-GB2584	W	20030617		

OTHER SOURCE(S):

MARPAT 140:41910

GI

Title compds. I [n = 0-2; R1 = halo, alkyl, alkoxy, etc.; R2 = alkyl; Y = 1]AB absent, CH2; X = O, S] are prepared For instance, N-benzyl-N-hexyl-3-(4hydroxyphenyl)propanamide (preparation given) is reacted with Me 2-(bromomethyl)benzoate (CH3CN, K2CO3, 66°) and the product saponified (THF/H2O, LiOH, microwave, 120°, 40 min) to give II. Example compds. have EC50 < 50 μ mol/L for PPAR- α . I are useful for treating clin. conditions associated with insulin resistance. 637015-02-2P, 2-[[[4-[2-[(2,4-Difluorobenzyl)(heptyl)amino]-2-IT oxoethyl]phenyl]thio]methyl]benzoic acid 637015-05-5P, 2-[[4-[2-[Benzyl(hexyl)amino]-2-oxoethyl]phenoxy]methyl]benzoic acid 637015-07-7P, 2-[[4-[2-[(2,4-Difluorobenzyl)(heptyl)amino]-2oxoethyl]phenoxy]methyl]benzoic acid 637015-32-8P, 2-[[[4-[2-[Ethyl[4-(trifluoromethyl)benzyl]amino]-2oxoethyl]phenyl]thio]methyl]benzoic acid 637015-33-9P, 2-[[4-[2-[Ethyl(2-fluorobenzyl)amino]-2-oxoethyl]phenoxy]methyl]benzoic acid 637015-40-8P, 2-[[[4-[2-[(4-Chlorobenzyl)(ethyl)amino]-2oxoethyl]phenyl]thio]methyl]benzoic acid RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(ortho-substituted benzoic acid derivs. for treatment of insulin resistance)

RN 637015-02-2 HCAPLUS

CN Benzoic acid, 2-[[[4-[2-[[(2,4-difluorophenyl)methyl]heptylamino]-2-oxoethyl]phenyl]thio]methyl]- (9CI) (CA INDEX NAME)

$$CH_2-S$$
 CH_2-C-N
 CH_2
 C

RN 637015-05-5 HCAPLUS

CN Benzoic acid, 2-[[4-[2-[hexyl(phenylmethyl)amino]-2-oxoethyl]phenoxy]methyl]- (9CI) (CA INDEX NAME)

RN 637015-07-7 HCAPLUS

CN Benzoic acid, 2-[[4-[2-[[(2,4-difluorophenyl)methyl]heptylamino]-2-oxoethyl]phenoxy]methyl]- (9CI) (CA INDEX NAME)

RN 637015-32-8 HCAPLUS

CN Benzoic acid, 2-[[[4-[2-[ethyl[[4-(trifluoromethyl)phenyl]methyl]amino]-2-oxoethyl]phenyl]thio]methyl]- (9CI) (CA INDEX NAME)

CN Benzoic acid, 2-[[4-[2-[ethyl[(2-fluorophenyl)methyl]amino]-2-oxoethyl]phenoxy]methyl]- (9CI) (CA INDEX NAME)

RN 637015-40-8 HCAPLUS

CN Benzoic acid, 2-[[[4-[2-[[(4-chlorophenyl)methyl]ethylamino]-2-oxoethyl]phenyl]thio]methyl]- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:

2004:2679 HCAPLUS

DOCUMENT NUMBER:

140:76898

TITLE:

Preparation of benzoic acid derivatives as modulators

of PPAR- α and PPAR- γ

INVENTOR(S):

Li, Lanna

PATENT ASSIGNEE(S):

Astrazeneca AB, Swed.; Astrazeneca UK Limited

SOURCE:

PCT Int. Appl., 101 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.							APPLICATION NO.										
WO	2004								WO 2003-GB2598								
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,
		CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	ΚP,	KR,	KZ,	LC,	LK,	LR,
		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NI,	NO,	NZ,	OM,
		PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	TJ,	TM,	TN,	TR,
		TT,	TZ,	UA,	UG,	US,	UΖ,	VC,	VN,	ΥU,	ZA,	ZM,	ZW				
	RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	ŪĠ,	ZM,	ZW,	AM,	ΑZ,	BY,
		KG,	ΚZ,	MD,	RU,	ТJ,	TM,	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,
•		FI,	FR,	GB,	GR,	HU,	IE,	IT,	LU,	MC,	NL,	PT,	RO,	SE,	SI,	SK,	TR,
		BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	ΝE,	SN,	TD,	TG
CA 2490687			AA		2003	1231	CA 2003-2490687				20030617						
ΑU	AU 2003240101			A1	20040106			AU 2003-240101					20030617				
BR	BR 2003011840		Α	20050315			BR 2003-11840					20030617					
							EP 2003-732715										
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,
		IE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL,	TR,	BG,	CZ,	EE,	HU,	SK	
CN	CN 1662230			A	·	2005	0831					20030617					

JP 2006502105	T2	20060119	JР	2004-515010		20030617
NZ 536972	A	20060630	NZ	2003-536972		20030617
NO 2004005222	A	20050119	NO	2004-5222		20041129
ZA 2004009690	A	20051011	ZA	2004-9690		20041130
US 2005267149	A1	20051201	US	2004-518819		20041220
PRIORITY APPLN. INFO.:			SE	2002-1937	Α	20020620
			WO	2003-GB2598	W	20030617

OTHER SOURCE(S):

MARPAT 140:76898

GI

Title compds. I [R1 = (un) substituted aryl, alkyl, acyl, etc.; AB (CH2)m-T-(CH2)n-U-(CH2)p = attached at either the meta or para position(to V) and is O(CH2)2, O(CH2)3, etc.; V = O, S, amino, single bond; q =1-3; W = 0, S, amido, amino, single bond; R2 = halo, alkyl, alkoxy, etc.; r = 0-3; R3 = halo, alkyl, alkoxy, etc.; s = 0-3; with some provisions are prepared For instance, tert-Bu [3-[[[(1,1'-biphenyl-4yl)carbonyl]amino]methyl]phenyl]carbamate (preparation given) is deprotected (CH2Cl2, TFA) and alkylated with 3-carboxybenzaldehyde (HOAc, NaBH4) to give II. Compds. of the invention have an EC50 < 50 \mumol/L for PPAR- α and PPAR- γ . I are useful in treating clin. conditions associated with insulin resistance. 637358-56-6P, 2-[[4-[2-[Benzyl(hexyl)amino]-2-oxoethyl]-2-IT fluorophenoxy]methyl]benzoic acid 637358-59-9P, 2-[[4-{2-[Benzyl (hexyl) amino]-2-oxoethyl]-2-methoxyphenoxy]methyl]benzoic RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of benzoic acid derivs. as modulators of PPAR- α and $PPAR-\gamma)$

637358-56-6 HCAPLUS

RN

10/518,007

CN Benzoic acid, 2-[[2-fluoro-4-[2-[hexyl(phenylmethyl)amino]-2-oxoethyl]phenoxy]methyl]- (9CI) (CA INDEX NAME)

Me- (CH₂)₅-N-C-CH₂

Ph-CH₂

$$O$$

HO₂C

RN 637358-59-9 HCAPLUS

CN Benzoic acid, 2-[[4-[2-[hexyl(phenylmethyl)amino]-2-oxoethyl]-2-methoxyphenoxy]methyl]- (9CI) (CA INDEX NAME)

6

REFERENCE COUNT:

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT